

References where the mathematical symbols are defined:

The fragment molecular orbital method: practical applications to large molecular systems, D. G. Fedorov, K. Kitaura, Eds., CRC Press (2009), in press, chapter 1, or D. G. Fedorov, K. Kitaura, H. Li, J. H. Jensen, M. S. Gordon, J. Comp. Chem., 27 (2006) 976-985.

One-body FMO properties.

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	Ecorr	E'_I	Euncorr	DX	DY	DZ
1(frg00001,L1)	-76.198612403		-76.014638036	-1.78955	0.75817	1.64693
2(frg00002,L1)	-76.198948441		-76.015021402	1.36181	1.05519	-1.87377
3(frg00003,L1)	-76.198981340		-76.015065952	0.30259	-2.20909	-1.22534

Total energy of the molecule: Ecorr (1)= -228.596542184

Total energy of the molecule: Euncorr(1)= -228.044725390

Total energy of the molecule: Edelta (1)= -0.551816794

Dipole moment D(xyz),DA(1)= -0.1251576 -0.3957289 -1.4521729 1.5103218

Two-body FMO properties.

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DL: D=C dynamically correlated (MP2,CI), D=N not dynamically correlated

(RHF,DFT). D=S separated dimer: semiclassical interaction (ES), D=M MCSCF.

L stands for layer, Z is the monomer charge product, R is the interfragment distance relative to van-der-Waals radii (-1.00 is printed if distances are not computed). dDIJ*VIJ is the density polarisation contribution.

Q(I->J) is the charge transfer amount, printed as zero if not available.

Positive values correspond to I in IJ having extra negative charge.

I	J	DL	Z	R	Q(I->J)	Ecorr	Euncorr	EIJ-EI-EJ,corr/uncorr	dDIJ*VIJ,unc tot,corr	
				R_{IJ}	ΔQ_{IJ}			$\Delta E'_{IJ}$	$\Delta E'^{RHF}_{IJ}$	$Tr(\Delta \mathbf{D}^{IJ} \mathbf{V}^{IJ})$
										ΔE^{int}_{IJ}
2	1	C1	0	0.76	0.0285	-152.411283188	-152.040818007	-0.01372234	-0.01115857	-0.00074728
3	1	C1	0	0.76	-0.0276	-152.411322427	-152.040901722	-0.01372868	-0.01119773	-0.00072459
3	2	C1	0	0.77	0.0255	-152.410247039	-152.039969786	-0.01231726	-0.00988243	-0.00068220

Total energy of the molecule: Ecorr (2)= -228.638464541 $E^{FMO2-MP2}$

Total energy of the molecule: Euncorr(2)= -228.079118197 $E^{FMO2-RHF}$

Total energy of the molecule: Edelta (2)= -0.559346345

Dipole moment D(xyz),DA(2)= -0.1472843 -0.3832508 -1.4534028 1.5102826 $\mathbf{D}^{FMO2-RHF}$

Charge transfer for each fragment:

IFG QFG DeltaQ and its contributions from JFG, Q(JFG->IFG).

1	0	0.0009	=	2->	0.0285	3->	-0.0276
2	0	-0.0030	=	1->	-0.0285	3->	0.0255
3	0	0.0021	=	1->	0.0276	2->	-0.0255

Total absolute monomer transf. charge = 0.006060 $\Delta \bar{Q}$

Total amount of absolute transf. charge = 0.081689 ΔQ

FMO-PCM properties.

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Ges is the energy of electrostatic interaction,
included in the individual n-mer and total FMO energies.
Internal energies are for solute only excluding all interactions with solvent.

I	Ges	Gcav	Gdisp	Grep (all in kcal/mol)
1 (frg00001)	-4.957	3.670	-4.059	1.113
2 (frg00002)	-5.176	3.678	-4.080	1.122
3 (frg00003)	-5.236	3.676	-4.101	1.129

Total Ges(1)= -15.369 kcal/mol.

I	J	Ges,	dGes (kcal/mol)
2	1	-10.118	0.015
3	1	-10.188	0.005
3	2	-10.401	0.011

Total Ges(2)= -15.338 kcal/mol.

ELECTROSTATIC INTERACTION	=	-15.338 KCAL/MOL	ΔG_{es}
PIEROTTI CAVITATION ENERGY	=	11.024 KCAL/MOL	ΔG_{cav}
DISPERSION FREE ENERGY	=	-12.240 KCAL/MOL	ΔG_{disp}
REPULSION FREE ENERGY	=	3.364 KCAL/MOL	ΔG_{rep}
TOTAL INTERACTION	=	-13.190 KCAL/MOL	$\Delta G_{es} + \Delta G_{cav} + \Delta G_{disp} + \Delta G_{rep}$

Free corr. energy in solvent= -228.635041424 $G_{FMO2-MP2/PCM} = E_{FMO2-MP2/PCM} + \Delta G_{cav} + \Delta G_{disp} + \Delta G_{rep}$
Internal corr. energy in solvent= -228.614021800 $G'_{FMO2-MP2/PCM} = G_{FMO2-MP2/PCM} - (\Delta G_{es} + \Delta G_{cav} + \Delta G_{disp} + \Delta G_{rep})$

Free uncorrelated energy in solvent= -228.075695079 $G_{FMO2-RHF/PCM}$
Internal uncorrelated energy in solvent= -228.054675455 $G'_{FMO2-RHF/PCM}$

n-body Mulliken atomic charges Q(n)

IAT	IFG	Z	Q(1)	Q(2)	Q(3)
1	1	8.0	-0.999729	-1.002453	
2	1	1.0	0.500836	0.509644	
3	1	1.0	0.498893	0.493733	
4	2	8.0	-0.998937	-1.004276	
5	2	1.0	0.499763	0.507704	
6	2	1.0	0.499174	0.493542	
7	3	8.0	-0.999854	-1.000967	
8	3	1.0	0.500201	0.508502	
9	3	1.0	0.499653	0.494571	